

SELECTION OF COORDINATION GEOMETRY TO ADJUST WATER EXCHANGE RATES
OF PARAMAGNETIC METAL ION-BASED MACROCYCLIC CONTRAST AGENTS

ABSTRACT OF THE DISCLOSURE

The present invention is directed, in general, to a contrast agent comprising a tetraazacyclododecane ligand and comprising a macrocyclic ring and a paramagnetic metal ion coordinated to the tetraazacyclododecane ligand. Pendant arms R, R', R'' and R''' attached to a ring nitrogen. The pendant arms have the general formula: $-C'HR^1R^2$ and for three or more of the pendant arms a chirality of the carbon atoms C' are identical for each of three or more of the pendant arms. The R^1 group is larger than hydrogen and R^2 is selected from the group consisting of: an alcohol, amides, a carboxylate, phosphinates and a phosphonate. One or more substituents R^6 is a group larger than a methyl group and is located on one or more ring carbons. Other embodiments of the invention include a method of using the contrast agent and a water molecule (H_2O) associated with the tetraazacyclododecane ligand to obtain a magnetic resonance signal by applying a radio frequency pulse at about a resonance frequency of water. Still other embodiments of the invention include a magnetic resonance system comprising the contrast agent and associated H_2O , and a magnetic resonance apparatus configured to produce a radio-frequency pulse that causes the contrast agent to produce a magnetic resonance signal.